Sub-Nanostructured Non-Transition Metal Complex Grids for Hydrogen Storage (New FY 2004 Project)

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Objectives

To grow sub-nanostructured metal grids for hydrogen absorption in storage applications

Technical Barriers

This project addresses the following technical barrier from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year R,D&D Plan:

- M. Hydrogen Capacity and Reversibility

Approach

The primary goal of this project is to grow sub-nanostructured metal grids for hydrogen absorption in storage applications. Sub-nanostructuring will:

1. Increase hydrogen molecule dissociation rate on the active sites
2. Increase hydrogen atom transport rate into the metal
3. Decrease performance degradation by cycling caused by decrepitation
4. Increase heat transfer in the metal matrix
5. Increase hydrogen uptake

This novel approach involves electrochemically growing the metal phase, an atom at a time, in a sub-nanostructured "mold." The mold will be made from known zeolites including the recently discovered titanium silicate, which has unique structural characteristics. The energy required for the growth is minimal; it is equal to the electron charge (times the valence) per metal atom.

The major tasks involved in this project are: 1) zeolite growth and treatment, 2) cathode preparation, 3) electrochemical growth, 4) physical characterization, 5) chemical characterization and performance evaluation.

Task 1. Zeolite Growth and Treatment: It is necessary to grow zeolite crystals with the required morphology to obtain a uniform film on the cathode. Normal growth of zeolites involves hydrothermal synthesis between 150-300^{o}C under autonomous pressure in autoclaves. The crystal morphology is controlled by the solution chemistry (which may include inert additives) and time-temperature combination. The alumina/silica ratio of zeolites is controlled during synthesis to optimize the density of exchangeable cations. In addition to morphology, the formulations must be optimized for optimum cation density and for ease of zeolite mold removal after the metal grids are grown.

Task 2. Cathode Preparation: Cathode preparation is the most significant technical hurdle in this project. The cathode coated with zeolites must not have any macroscopic pathway for cations to diffuse. This requires mechanical compacting and/or polymer patching and/or in-situ growth of the zeolite around the electrode. We will start with readily available powders in our labs to gain experience in cathode preparation. Later, we will switch to specially grown powders in Task 1 to minimize the macropores.

Task 3. Electrochemical Growth: This is the heart of the process, where the metal grid is electrochemically grown in the zeolite micropores one atom at a time. We will start electrochemical growth with electrodes prepared by mechanical compaction with readily available powders to gain experience with electrochemical growth. Later, we will switch to specially prepared electrodes. In all cases, the growth kinetics will be closely monitored.

Task 4. Physical Characterization: The metal grids will be first physically characterized by using standard techniques such as optical and scanning electron microscopy for morphology, x-ray fluorescence for non-destructive and wet-chemistry including atomic absorption as destructive elemental analysis, atomic force mocroscopy/scanning tunneling microscopy for nano-structure analysis, and simple density measurements. Only samples that show acceptable nano-structure will be chemically characterized after zeolite mold removal.

Task 5. Chemical Characterization and Performance Evaluation: Analysis of equilibrium and kinetic data coupled with physical property data enable hydrogen storage performance calculations including mass balances, energy balances, estimated charge/discharge times (under isothermal conditions), etc. The performance calculations will be based on the packing material rather than the overall system. The performance will be compared to available data for other approaches and to the target values.

During the first year of the project, it will be determined whether pure metal grids can be grown that have equilibrium and/or kinetic performance better than the same metal in bulk phase. In the second year, the cathode preparation method will be finalized, and sub-nanostructured non-transition metal complex grids will be grown. In the third year, anode preparation and electrolyte chemistry will be finalized, an analysis will be completed of projected hydrogen storage, and an evaluation/cost estimate will be completed.